Atilla Bende

List of Publications by Year
in descending order

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88	1,467	623734	345221
papers	citations	14 h-index	36 g-index

88	88	88	2549
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Photoionization, Structures, and Energetics of Naâ€Doped Formic Acidâ€“Water Clusters. ChemPhysChem, 2022, 23, .	2.1	2
2	Study of Mixed Clusters of Water and N,N'-dimethylethyleneurea. Ukrainian Journal of Physics, 2022, 56, 796.	0.2	1
3	Dopamine Photochemical Behaviour under UV Irradiation. International Journal of Molecular Sciences, 2022, 23, 5483.	4.1	7
4	Theoretical modeling of the singletâ€“triplet spin transition in different Ni(<scp>ii</scp>)-diketo-pyrphyrin-based metalâ€“ligand octahedral complexes. Physical Chemistry Chemical Physics, 2021, 23, 4784-4795.	2.8	1
5	An attempt to synthesize a terthienyl-based analog of indacenedithiophene (IDT): unexpected synthesis of a naphtho[2,3-b]thiophene derivative. RSC Advances, 2021, 11, 9894-9900.	3.6	1
6	The Influence of UV Femtosecond Laser Pulses on Bacterial DNA Structure, as Proved by Fourier Transform Infrared (FTâ€IR) Spectroscopy. ChemistrySelect, 2021, 6, 6957-6972.	1.5	5
7	Halogen-Bonded Organic Frameworks of Perfluoroiodo- and Perfluorodiiodobenzene with 2,2â€²,7,7â€²-Tetrapyridyl-9,9â€²-spirobifluorene. Crystal Growth and Design, 2021, 21, 1045-1054.	3.0	11
8	"The full mapping of low-lying excited state relaxation dynamic pathways for acetophenone ". Studia Universitatis Babes-Bolyai Chemia, 2021, 66, 239-253.	0.2	0
9	Theoretical Study of Light-Induced Crosslinking Reaction Between Pyrimidine DNA Bases and Aromatic Amino Acids. Frontiers in Bioengineering and Biotechnology, 2021, 9, 806415.	4.1	2
10	Synthesis, Structure and Supramolecular Properties of a Novel C3 Cryptand with Pyridine Units in the Bridges. Molecules, 2020, 25, 3789.	3.8	2
11	Sugar matters: sugar moieties as reactivity-tuning factors in quercetin O-glycosides. Food and Function, 2020, 11, 5293-5307.	4.6	12
12	Calculations of electron transfer in the tris[4-(2-thienyl)phenyl]amineâ€“C70 donor-acceptor system. Chemical Physics Letters, 2020, 754, 137654.	2.6	1
13	The influence of monovalent and divalent metal cations on the stability of the DNA-protein interaction in the nucleosome core particle. Advances in Quantum Chemistry, 2020, , 269-290.	0.8	1
14	Halogen Bonds (N···I) at Work: Supramolecular Catemeric Architectures of 2,7-Dipyridylfluorene with ortho-, meta-, or para-Diiodotetrafluorobenzene Isomers. Crystal Growth and Design, 2020, 20, 3429-3441.	3.0	17
15	Clusters tagged by alkali metals. AIP Conference Proceedings, 2020, , .	0.4	2
16	DFT study of adiabatic singlet-triplet energy gaps in Ni(II)-based macrocyclic-ligand supramolecular complexes. AIP Conference Proceedings, 2020, , .	0.4	2
17	Exploring the Polymorphism of Drostanolone Propionate. Molecules, 2020, 25, 1436.	3.8	10
18	Design, synthesis and structure of novel dendritic G-2 melamines comprising piperidine motifs as key linkers and 4-(n-octyloxy)aniline as a peripheral unit. Tetrahedron, 2019, 75, 130468.	1.9	0

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19	Intermolecular Interaction in Methylene Halide (CH2F2, CH2Cl2, CH2Br2 and CH2I2) Dimers. Molecules, 2019, 24, 1810.	3.8	6
20	Light-induced spin transitions in Ni(II)-based macrocyclic-ligand complexes: A DFT study. Journal of Photochemistry and Photobiology A: Chemistry, 2019, 376, 316-323.	3.9	8
21	Improving the Light-Induced Spin Transition Efficiency in Ni(II)-Based Macrocyclic-Ligand Complexes. Molecules, 2019, 24, 4249.	3.8	5
22	Succinic, fumaric, adipic and oxalic acid cocrystals of promethazine hydrochloride. Acta Crystallographica Section C, Structural Chemistry, 2019, 75, 107-119.	0.5	6
23	Poly[3,4â€dihydroxybenzhydrazide]: A Polydopamine Analogue?. Macromolecular Chemistry and Physics, 2018, 219, 1700564.	2.2	7
24	Graphene-porphyrin composite synthesis through graphite exfoliation: The electrochemical sensing of catechol. Sensors and Actuators B: Chemical, 2018, 256, 665-673.	7.8	46
25	A three-armed cryptand with triazine and pyridine units: synthesis, structure and complexation with polycyclic aromatic compounds. Beilstein Journal of Organic Chemistry, 2018, 14, 1370-1377.	2.2	2
26	UV Photoionization of Sodiumâ€Doped Formic Acid Clusters. ChemPhysChem, 2018, 19, 2724-2734.	2.1	4
27	Design, synthesis and structure of novel G-2 melamine-based dendrimers incorporating 4-(n-octyloxy)aniline as a peripheral unit. Beilstein Journal of Organic Chemistry, 2018, 14, 1704-1722.	2.2	3
28	The nature of intermolecular interactions in pyridiniumâ€“anionâ€“Î²-hexachlorocyclohexane molecular crystals. Physical Chemistry Chemical Physics, 2017, 19, 20691-20698.	2.8	9
29	New p-aminophenol-based dendritic melamines. Iterative synthesis, structure, and electrochemical characterisation. Comptes Rendus Chimie, 2017, 20, 402-414.	0.5	2
30	Low-lying excited states and their relaxation pathways of phenothiazine. AIP Conference Proceedings, 2017, , .	0.4	0
31	Supramolecular anion recognition by Î²-HCH. Chemical Communications, 2016, 52, 12322-12325.	4.1	9
32	Glassy carbon electrode modified with hemin and new melamine compounds for H2O2 amperometric detection. Journal of Solid State Electrochemistry, 2016, 20, 3071-3081.	2.5	9
33	Encasing of Na⁺ ion in dimerâ€formed acetic acid clusters. Journal of Mass Spectrometry, 2015, 50, 1136-1143.	1.6	3
34	Inception of Acetic Acid/Water Cluster Growth in Molecular Beams. ChemPhysChem, 2015, 16, 3021-3029.	2.1	7
35	Modeling Laser-Induced Molecule Excitations Using Real-Time, Time-Dependent Density Functional Theory. Annual Reports in Computational Chemistry, 2015, 11, 103-146.	1.7	1
36	Synthesis, structure, electrochemical behaviour and electrochemical investigations on the assembling with pyrene of a novel C3 cryptand. Supramolecular Chemistry, 2015, 27, 52-58.	1.2	3

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37	Modeling laser induced molecule excitation using real-time time-dependent density functional theory: application to 5- and 6-benzyluracil. Physical Chemistry Chemical Physics, 2015, 17, 5861-5871.	2.8	10
38	Theoretical investigation of polymer chain stability in the metal coordinated azorubine and cyclam complex. Chemical Physics, 2015, 457, 152-159.	1.9	4
39	Exotic Allotropes of Carbon. Carbon Materials, 2015, , 185-201.	1.2	2
40	Tautomerism and proton transfer in photoionized acetaldehyde and acetaldehydeâ€“water clusters. Journal of Mass Spectrometry, 2014, 49, 700-708.	1.6	7
41	The influence of anharmonic and solvent effects on the theoretical vibrational spectra of the guanineâ€“cytosine base pairs in Watsonâ€“Crick and Hoogsteen configurations. Journal of Molecular Modeling, 2014, 20, 2113.	1.8	6
42	Carbon multi-shell cages. Physical Chemistry Chemical Physics, 2014, 16, 5260.	2.8	8
43	Dressed Adiabatic and Diabatic Potentials To Study Topological Effects for F + H₂. Journal of Physical Chemistry A, 2014, 118, 6361-6366.	2.5	13
44	Quantum molecular biological investigation of the onset of cancer. International Journal of Quantum Chemistry, 2014, 114, 1229-1235.	2.0	3
45	Influence of the sequence on the ab initio band structures of single and double stranded DNA models. Physics Letters, Section A: General, Atomic and Solid State Physics, 2014, 378, 2157-2162.	2.1	9
46	Structure of Polydopamine: A Never-Ending Story?. Langmuir, 2013, 29, 10539-10548.	3.5	834
47	Hole mobilities of periodic models of DNA double helices in the nucleosomes at different temperatures. Chemical Physics Letters, 2013, 565, 128-131.	2.6	6
48	Vacuum ultraviolet photoionization and ab initio Investigations of methyl tert-butyl ether (MTBE) clusters and MTBEâ€“water clusters. Chemical Physics Letters, 2013, 561-562, 18-23.	2.6	4
49	Diamond and Related Nanostructures. Carbon Materials, 2013, , .	1.2	14
50	Low-lying excited-states of 5-benzyluracil. Physical Chemistry Chemical Physics, 2013, 15, 7161.	2.8	14
51	A tri-atomic Renner-Teller system entangled with Jahn-Teller conical intersections. Journal of Chemical Physics, 2013, 138, 024113.	3.0	16
52	Dressed Adiabatic and Diabatic Potentials for the Rennerâ€“Teller/Jahnâ€“Teller F + H₂ System. Journal of Physical Chemistry A, 2013, 117, 8497-8505.	2.5	9
53	Low-lying excited-states and relaxation pathways of acetophenone. , 2013, , .		0
54	Energetics of Multi-shell Cages. Carbon Materials, 2013, , 107-119.	1.2	1

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55	Solvent effect on the anharmonic vibrational frequencies in guanine-cytosine base pair. , 2012, , .		1
56	Chitosan-based nanocarriers for antimalarials. , 2012, , .		1
57	Study of binary systems of Î²-cyclodextrin with a highly potential anti-mycobacterial drug. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2012, 74, 129-135.	1.6	5
58	On diamond D5. Structural Chemistry, 2012, 23, 981-986.	2.0	12
59	Possible role of ions in DNAâ€“protein interactions in the nucleosomes. Chemical Physics Letters, 2012, 525-526, 115-119.	2.6	3
60	Complexation of Amlodipine Besylate with Î²-Cyclodextrin. Acta Chimica Slovenica, 2012, 59, 18-23.	0.6	2
61	Weakly bonded cluster structures of N,Nâ€²-dimethylethyleneurea and water. Journal of Molecular Liquids, 2011, 162, 45-49.	4.9	2
62	Localization and anharmonicity of the vibrational modes for GC Watsonâ€“Crick and Hoogsteen base pairs. Journal of Molecular Modeling, 2011, 17, 3265-3274.	1.8	7
63	Structural investigation of chitosan-based microspheres with some anti-inflammatory drugs. Journal of Molecular Structure, 2011, 997, 78-86.	3.6	13
64	Ab initio structures of interacting methylene chloride molecules with comparison to the liquid phase. Journal of Molecular Liquids, 2011, 158, 205-207.	4.9	3
65	Model calculations of the energy band structures of double stranded DNA in the presence of water and Na+ ions. Solid State Communications, 2011, 151, 301-305.	1.9	10
66	Nitrogen Substituted Phenothiazine Derivatives: Modelling of Molecular Self-Assembling. International Journal of Molecular Sciences, 2011, 12, 3102-3116.	4.1	5
67	Charge transfer between DNA and proteins in the nucleosomes. Theoretical Chemistry Accounts, 2010, 125, 185-191.	1.4	4
68	Hydrogen bonding in the urea dimers and adenineâ€“thymine DNA base pair: anharmonic effects in the intermolecular H-bond and intramolecular H-stretching vibrations. Theoretical Chemistry Accounts, 2010, 125, 253-268.	1.4	27
69	Photoionisation and structures of jet-formed toluene clusters. Chemical Physics Letters, 2010, 495, 17-23.	2.6	14
70	Model calculation of the specific hole conductivities of three homopolynucleotides, poly(guanilic) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 Communications, 2010, 150, 446-449.	1.9	0
71	Omega Polynomial in Diamond-like Networks. Fullerenes Nanotubes and Carbon Nanostructures, 2010, 18, 236-243.	2.1	8
72	Molecular Modeling of Phenothiazine Derivatives: Self-Assembling Properties. Journal of Physical Chemistry A, 2010, 114, 12479-12489.	2.5	16

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73	A simple model for the band structure and D.C. conductivity of an infinite Cï£¾OÂ·Â·Â·Hï£¿N chain perpendicular to the protein backbone. International Journal of Quantum Chemistry, 2009, 109, 612-617.	2.0	2
74	Circulene covered fullerenes. Computational and Theoretical Chemistry, 2009, 904, 28-34.	1.5	8
75	H-Bond-Driven Supramolecular Architectures of the Syn and Anti Isomers of the Dioxime of Bicyclo[3.3.1]nonane-3,7-dione. Journal of Organic Chemistry, 2009, 74, 3944-3947.	3.2	12
76	Molecular modeling of the weakly bounded dimers of some phenothiazine derivatives. Journal of Physics: Conference Series, 2009, 182, 012001.	0.4	0
77	The role of water and K+ ion in the charge transfer between <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.gif" display="inline" overflow="scroll"><mml:mrow><mml:msubsup><mml:mrow><mml:mtext>PO</mml:mtext></mml:mrow><mml:mrow><mml:mn>4</mml:mn></mml:mrow> groups of DNA and the lysine+ and arginine+ side chains of histone proteins. Chemical Physics Letters, 2008, 463, 211-213.	2.0	11
78	Weak intermolecular bonding in N,Nâ€²-dimethylethyleneurea dimers and N,Nâ€²-dimethylethyleneureaâ€“water systems: The role of the dispersion effects in intermolecular interaction. Chemical Physics, 2008, 354, 202-210.	1.9	12
79	ITIM distributed grid system applied in high energy, biomolecular and nanotehnology physics. , 2008, , .		2
80	The electronic structure of the four nucleotide bases in DNA, of their stacks, and of their homopolynucleotides in the absence and presence of water. Journal of Chemical Physics, 2008, 128, 105101.	3.0	21
81	Calculation of the hole mobilities of the three homopolynucleotides, poly(guanilic acid), poly(adenilic acid), and polythymidine in the presence of water andNa+ions. Physical Review E, 2008, 78, 061923.	2.1	4
82	Calculation of the band structure of polyguanilic acid in the presence of water and Na+ ions. Journal of Chemical Physics, 2007, 127, 055102.	3.0	16
83	Charge transfer between the <mml:math altimg="si3.gif" display="inline" overflow="scroll" xmlns:xocs="http://www.elsevier.com/xml/xocs/dtd" xmlns:xs="http://www.w3.org/2001/XMLSchema" xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" xmlns="http://www.elsevier.com/xml/ja/dtd" xmlns:ja="http://www.elsevier.com/xml/ja/dtd" xmlns:mml="http://www.w3.org/1998/Math/MathML" xmlns:tb="http://www.elsevier.com/xml/common/table/dtd" xmlns:sb="http://www.elsevier.com/xml/common/struct-bib/dtd" xmlns:ce="http://www... Chemical Phys...	2.6	11
84	Theoretical study of hydrogen bonds between acetylene and selected proton donor systems. International Journal of Quantum Chemistry, 2005, 101, 186-200.	2.0	3
85	BSSE-corrected geometry and harmonic and anharmonic vibrational frequencies of formamide-water and formamide-formamide dimers. International Journal of Quantum Chemistry, 2005, 103, 841-853.	2.0	31
86	Ab initio study of the ammonia-ammonia dimer: BSSE-free structures and intermolecular harmonic vibrational frequencies. International Journal of Quantum Chemistry, 2004, 99, 585-593.	2.0	9
87	BSSE-free description of intermolecular force constants in hydrogen fluoride and water dimers. International Journal of Quantum Chemistry, 2003, 92, 152-159.	2.0	14
88	BSSE-free description of the formamide dimers. International Journal of Quantum Chemistry, 2001, 84, 617-622.	2.0	15